

CRYSTAL DATA ON THE RADIOPROTECTANTS, N-(2-MERCAPTOPROPIONYL) GLYCINE AND N, N, N', N'-TETRAMETHYL-1,4-PHENYLENE DIAMINE-DIHYDROCHLORIDE

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N-(2-mercapto-propionyl) glycine, (MPG), (I) and N,N,N',N'-tetramethyl-1, 4-phenylene diamine, (TMPD), (II), are known^{1,2} to afford protection against ionising radiation. As part of a programme of 'x-ray investigations on chemical radioprotectants', we have crystallized MPG and the dihydrochloride of TMPD by slow evaporation from aqueous solutions. Both the compounds were found to have two crystal

forms each. The two different types of crystals crystallize simultaneously in the same crystallization dish, in each case. The unit cell dimensions and space group of the four types of crystals were determined from oscillation and Weissenberg photographs taken with CuK α radiation and the crystal data are listed in table I. Type 1 crystals of MPG correspond to a racemic mixture, whereas the type 2 crystals crystallizing in the space group P₂₁ contain only one kind of optical isomer which must have separated out during crystallization.

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1. Uma Devi, P., Saini, M. R., Verma, A. and Saharan, B. R., *Indian, J. Exp. Biol.*, 1978, **16**, 86.
2. Greenstock, G. L., Chapman, J. D., Raleigh, J. A., Shierman, E., and Reuvers, A. P., *Radn. Res.*, 1974, **59**, 556.
3. Vedavathi, B. M. and Vijayan, K., *Acta Cryst.*, 1981, B37, 475 and the references therein.

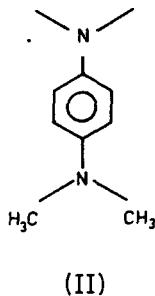
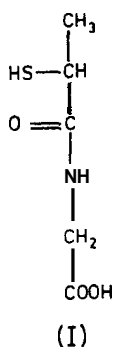


TABLE 1
Crystal data on MPG and TMPD di HCl

	MPG		TMPD diHCl	
	Formula C ₅ H ₉ NO ₃ S Molecular weight 163.2		Formula C ₁₀ H ₁₆ N ₂ . 2HCl Molecular weight 237.2	
	Type 1	Type 2	Type 1	Type 2
Crystals	Transparent, needle-like	Transparent, platy	Transparent, platy	Transparent, platy
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic
a	441 ± 0.01 Å	12.15 ± 0.03 Å	4.70 ± 0.01 Å	7.22 ± 0.02 Å
b	14.16 ± 0.01	5.20 ± 0.02	7.03 ± 0.02	4.82 ± 0.02
c	5.99 ± 0.01	5.50 ± 0.02	9.50 ± 0.01	18.88 ± 0.02
α			79.0 ± 1°	
β	121.2 ± 1°	114.1 ± 1°	87.0 ± 1°	114.0 ± 1°
γ			74.0 ± 1°	
Density (calc)	1.690 g.cm ⁻³	1.707 g.cm ⁻³	1.308 gm.cm ⁻³	1.199 gm.cm ⁻³
Density (expt)	1.64 ± 0.01 g.cm ⁻³	1.64 ± 0.01 g.cm ⁻³	1.265 ± 0.005 g.cm ⁻³	1.265 ± 0.0005 g.cm ⁻³
(Flotation in bromoform and ethyl acetate)			(Flotation in CCl ₄ and benzene)	
Z	2	2	1	2
Systematic absences	hol, l odd	oko, k odd	None	hol, h odd
Space group	Pc	P ₂ ₁	Pl or PP ₁	oko, k odd o and P ₂ ₁ /a

*The unit cell dimensions correspond to a positive reduced cell